BLUE WATERS

SUSTAINED PETASCALE COMPUTING

Model-Driven, Performance-Centric HPC Software and System Design and Optimization

Torsten Hoefler

With contributions from: William Gropp, William Kramer, Marc Snir

Scientific talk at Jülich Supercomputing Center

April 8th Jülich, Germany

GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

Imagine …

- … you're planning to construct a multi-million Dollar Supercomputer …
- … that consumes as much energy as a small [european] town …
- … to solve computational problems at an international scale and advance science to the next level …
- … with "hero-runs" of [insert verb here] scientific applications that cost $10k and more per run …

… and all you have (now) is …

- … then you better plan ahead!

Imagine …

- … you're designing a hardware to achieve 10^{18} operations per second …
- … to run at least some number of scientific applications at scale …
- … and everybody agrees that the necessary tradeoffs make it nearly impossible …
- ... where pretty much everything seems completely flexible (accelerators, topology, etc.) …

… and all you have (now) is …

- … how do you determine what the system needs to perform at the desired rate?
- … how do you find the best system design (CPU architecture and interconnection topology)?

State of the Art in HPC – A General Rant ☺

- Of course, nobody planned ahead ☺
- Performance debugging is purely empirical
  - Instrument code, run, gather data, reason about data, fix code, lather, rinse, repeat
- Tool support is evolving rapidly though!
  - Automatically find bottlenecks and problems
  - Usually done as black box! (no algorithm knowledge)
- Large codes are developed without a clear process
  - Missing development cycle leads to inefficiencies

Performance Modeling: State of The Art!

- Performance Modeling (PM) is done ad-hoc to reach specific goals (e.g., optimization, projection)
- But only for a small set of applications (the manual effort is high due to missing tool support)
- Payoff of modeling is often very high!
  - Led to the "discovery" of OS noise [SC03]
  - Optimized communication of a highly-tuned (assembly!) QCD code [MILC10] → >15% speedup!
  - Numerous other examples in the literature

[SC03]: Petrini et al. "The Case of Missing Supercomputer Performance …"
[MILC10]: Hoefler, Gottlieb: "Parallel Zero-Copy Algorithms for Fast Fourier Transform …"

Performance Optimization: State of the Art!

- Two major "modes":
  1. Tune until performance is sufficient for my needs
  2. Tune until performance is within X% of optimum
- Major problem: what is the optimum?
  - Sometimes very simple (e.g., Flop/s for HPL, DGEMM)
  - Most often not! (e.g., graph computations [HiPC'10])
- Supercomputers can be **very expensive!**
  - 10% speedup on Blue Waters can save millions $$$
  - Method (2) is generally preferable!

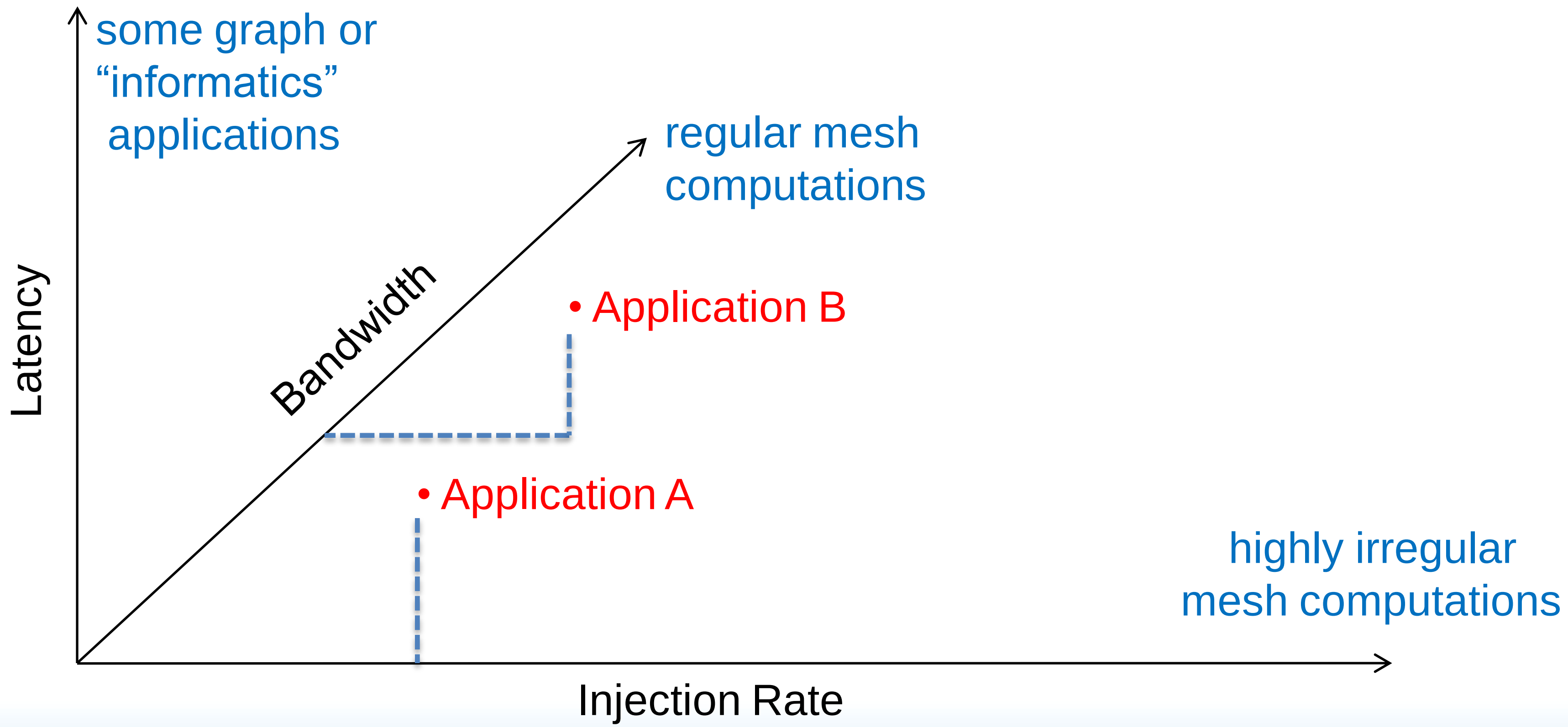
[HiPC'10]: Edmonds, Hoefler et al.: "A space-efficient parallel algorithm for computing Betweenness Centrality …

Ok, but what is this "Performance" about?

- Is it Flop/s?
  - Merriam Webster "flop: to fail completely"
- HPCC: MiB/s? GUPS? FFT-rate?
  - Yes, but more complex
  - Many (in)dependent features and metrics
    - network: bandwidth, latency, injection rate, …
    - memory and I/O: bandwidth, latency, random access rate, …
    - CPU: latency (pipeline depth), # execution units, clock speed, …
- Our very generic definition:
  - Machine model spans a vector space (feasible region)
  - Each application sits at a point in the vector space!

Example: Memory Subsystem (3 dimensions)

- Each application has particular coordinates



Our Practical and Simple Formalization

- Machine Model spans n-dimensional space $\Gamma = (p_1, p_2, \ldots, p_n)$
  - Elements are rates or frequencies (“operations per second”)
  - Determined from documentation or microbenchmarks
    - Netgauge’s memory and network tests [HPCC’07,PMEO’07]
- Application Model defines requirements $\tau = (r_1, r_2, \ldots, r_n)$
  - Determined analytically or with performance counters
  - Lower bound proofs can be very helpful here!
    - e.g., number of floating point operations, I/O complexity
- Time to solution (“performance”): $\max_{0<i\leq n}(r_i/p_i)$

[HPCC’07]: Hoefler et al.: “Netgauge: A Network Performance Measurement Framework”
[PMEO'07]: Hoefler et al: "Low-Overhead LogGP Parameter Assessment for Modern Interconnection Networks"

Should Parameter X be Included or Not?

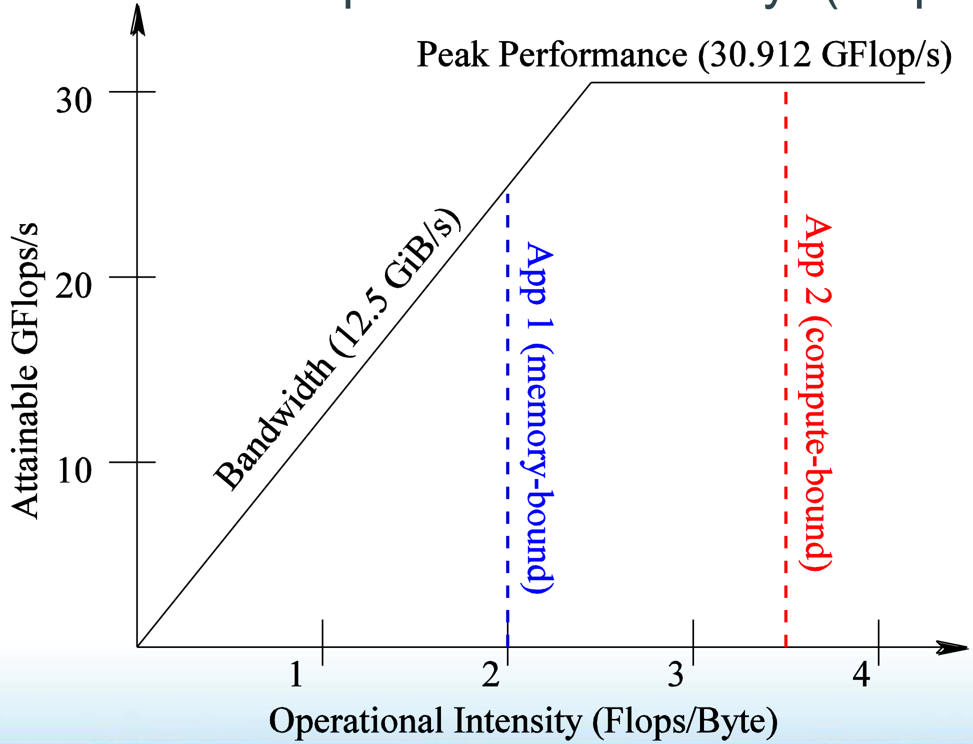
- The space is rather big (e.g., ISA instruction types!)

- Apply Occam's Razor wherever possible!
  - Einstein: "Make everything as simple as possible, but not simpler."
- Generate the simplest model for our purpose!
  - Not possible if not well understood, e.g., jitter [LSAP'10,SC10]

[SC10]: Hoefler et al.: "Characterizing the Influence of System Noise … by Simulation" (Best Paper)
[LSAP'10]: Hoefler et al.: "LogGOPSim – Simulating … Applications in the LogGOPS Model" (Best Paper)

A Pragmatic Example: The Roofline Model

- Only considers memory bandwidth and floating point rate but is very useful to guide optimizations! [Roofline]
  - Application model is "Operational Intensity" (Flops/Byte)



[Roofline] S. Williams et al.: "Roofline: An Insightful Visual Performance Model …"

The Roofline Model: Continued

- If an application reaches the roof: good!
- If not …
  - … optimize (vectorize, unroll loops, prefetch, …)
  - … **or** add more parameters!
    - e.g., graph computations, integer computations
- The roofline model is a special case in the "multi-dimensional performance space"
  - Picks two most important dimensions
  - Can be extended if needed!

[Roofline] S. Williams et al.: "Roofline: An Insightful Visual Performance Model …"

Caution: Resource Sharing and Parallelism

- Some dimensions might be "shared"
  - e.g., SMT threads share ALUs, cores share memory controllers, …
- Needs to be considered when dealing with parallelism (not just simply multiply performance)
  - Under investigation right now, relatively complex on POWER7

How to Apply this to Real Applications?

1. Performance-centric software development
   - Begin with a model and stick to it!
   - Preferred strategy, requires re-design

2. Analyze and model legacy applications
   - Use performance analysis tools to gather data
   - Form hypothesis (model), test hypothesis (fit data)

Performance-Centric Software Development

- Introduce Performance Modeling to all steps of the HPC Software Development Cycle:
  - Analysis (pick method, PM often exists [PPoPP’10])
  - Design (identify modules, re-use, pick algorithms)
  - Implementation (code in C/C++/Fortran - annotations)
  - Testing (correctness **and** performance! [HPCNano’06])
  - Maintenance (port to new systems, tune, etc.)

[HPCNano’06]: Hoefler et al.: “Parallel scaling of Teter's minimization for Ab Initio calculations”
[PPoPP'10]: Hoefler et al.: "Scalable Communication Protocols for Dynamic Sparse Data Exchange"

Tool 1: Performance Modeling Assertions

- Idea: The programmer adds model annotations to the source-code, the compiler injects code to:
  - Parameterize performance models
  - Detect anomalies during execution
  - Monitor and record/trace performance succinctly
- Has been explored by Alam and Vetter [MA'07]
  - Initial assertions and potential has been demonstrated!

[MA'07] Vetter, Alam: "Modeling Assertions: Symbolic Model Representation of Application Performance

Tool 2: Middleware Performance Models

- Algorithm choice can be complex
  - Especially with many unknowns, e.g.,
    - performance difference between reduce and allreduce?)
    - scaling of broadcast, it's **not** $O(S*\log_2(P))$
- Detailed models can guide early stages of software design but such modeling is hard
  - See proposed MPI models for BG/P in [EuroMPI'10]
  - Led to some surprises!

[EuroMPI'10]: Hoefler et al.: "Toward Performance Models of MPI Implementations …"

Example: Current Point-to-Point Models

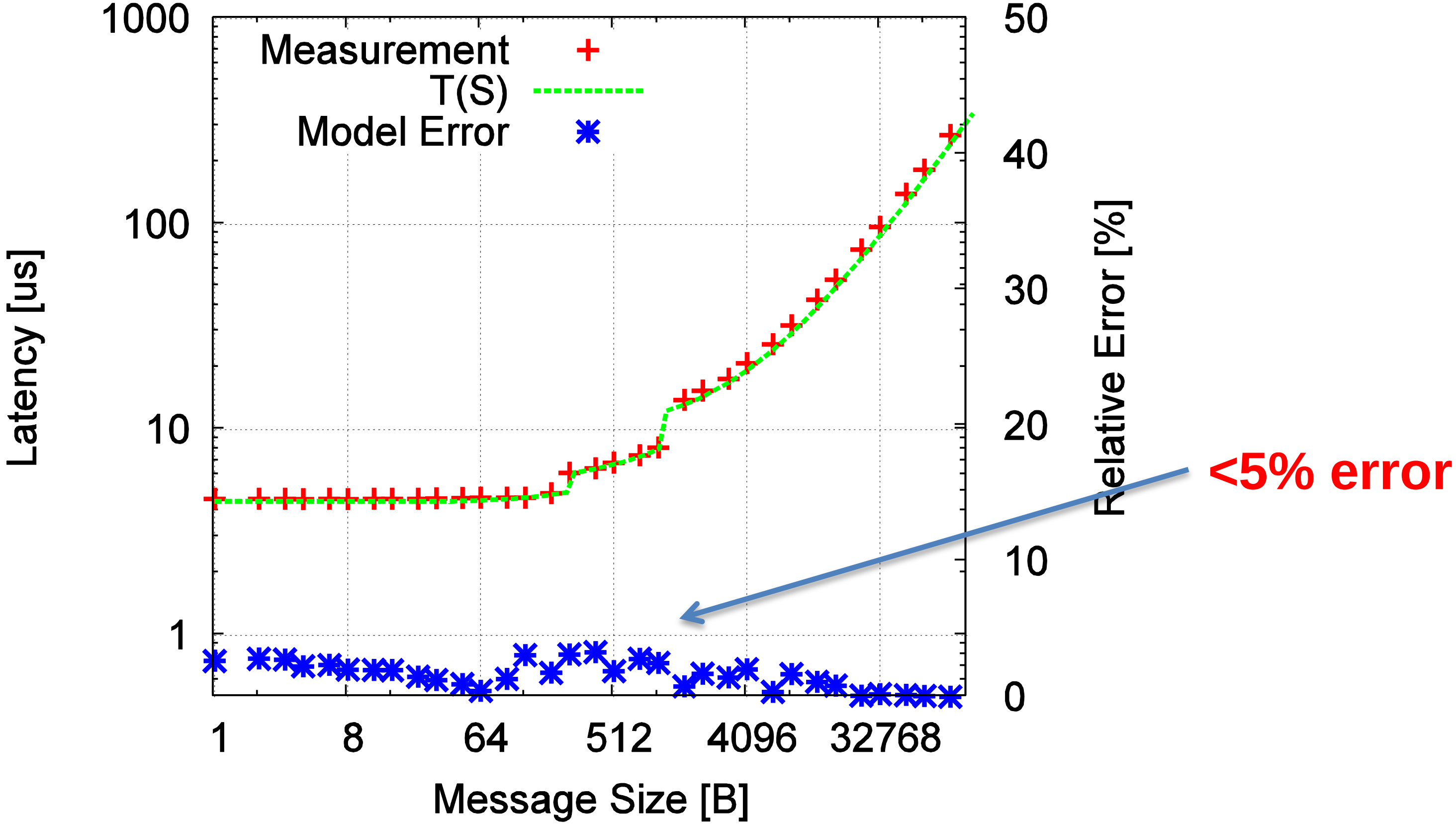
- Asymptotic (trivial): $\Theta(S)$
- Latency-bandwidth models: $T = \alpha + S\beta$
- Need to consider different protocol ranges
- Exact model for BG/P:

$$T(S) = \begin{cases} 4.5\mu s + 2.67ns/B \cdot S: & S \leq 256B \\ 5.7\mu s + 2.67ns/B \cdot S: & 256B < S \leq 1024B \\ 9.8\mu s + 2.67ns/B \cdot S: & 1024B < S \end{cases}$$

- Used Netgauge/logp benchmark
- Three ranges: small, eager, rendezvous

[EuroMPI'10]: Hoefler et al.: "Toward Performance Models of MPI Implementations …"

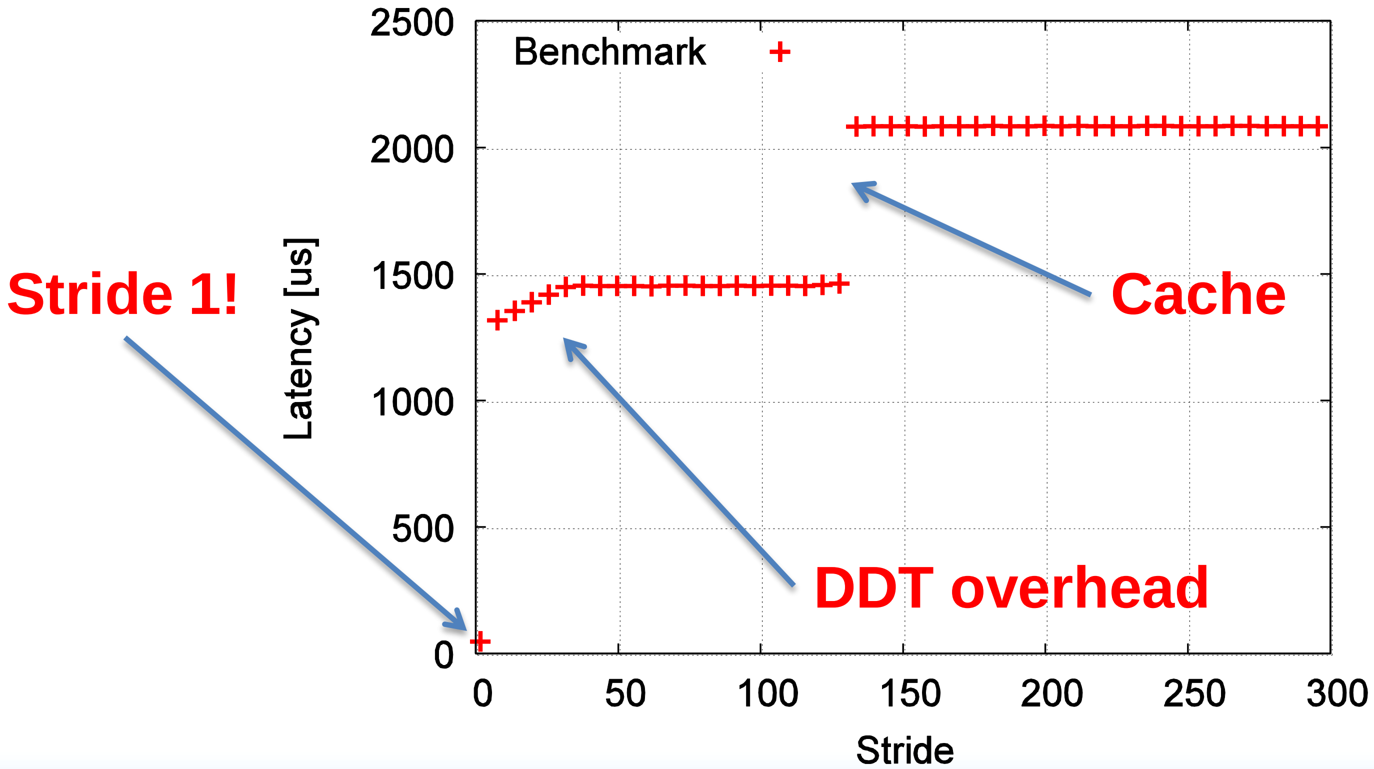
Example: Point-to-Point Model Accuracy



- Looks good, but there are problems!

Example: The not-so-ideal (but realistic) Case I

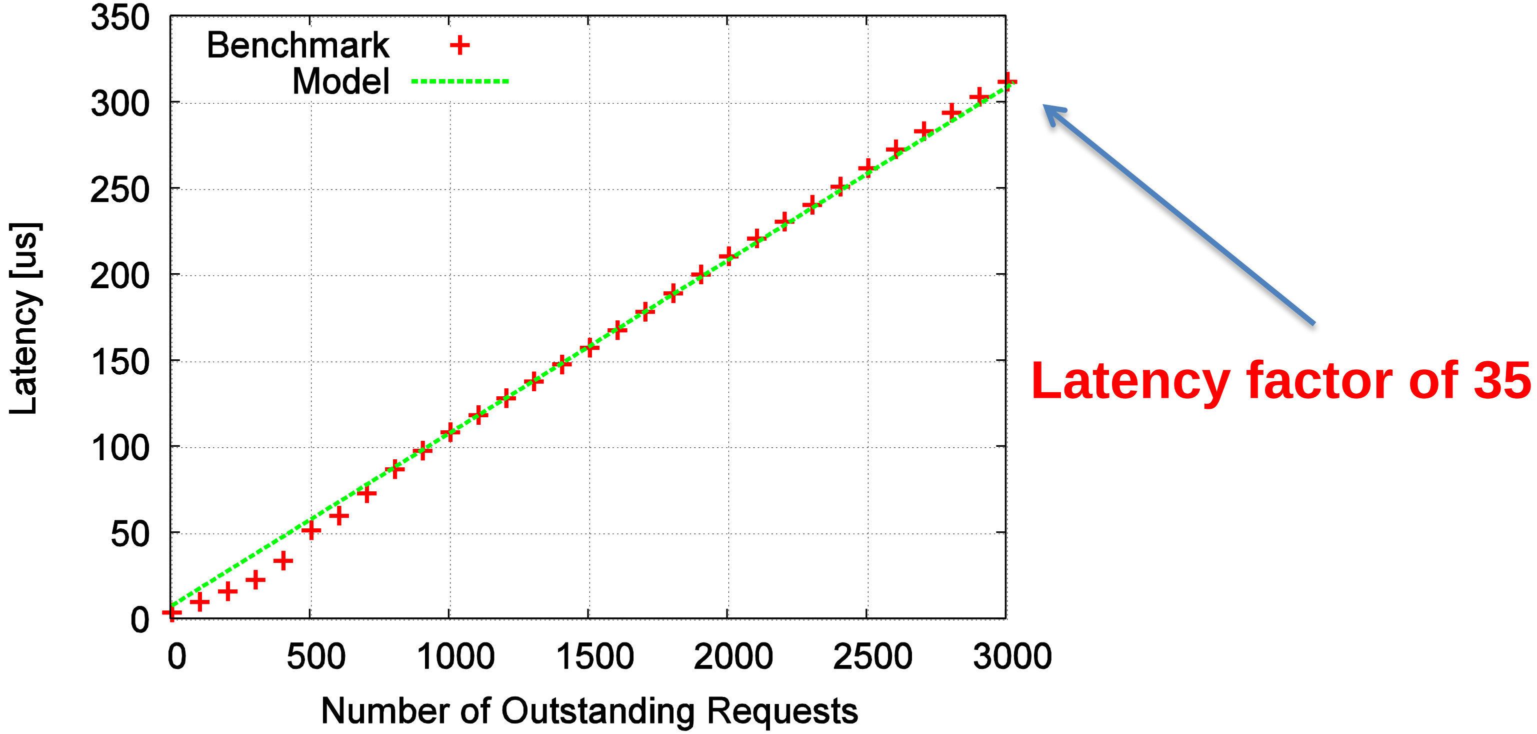
- Strided data-access (p2p model assumed stride-1)



- Benchmark: Netgauge: one_one_dtype, 16 kiB MPI_CHAR data

Example: The not-so-ideal (but realistic) Case II

- Matching queue overheads (very common)



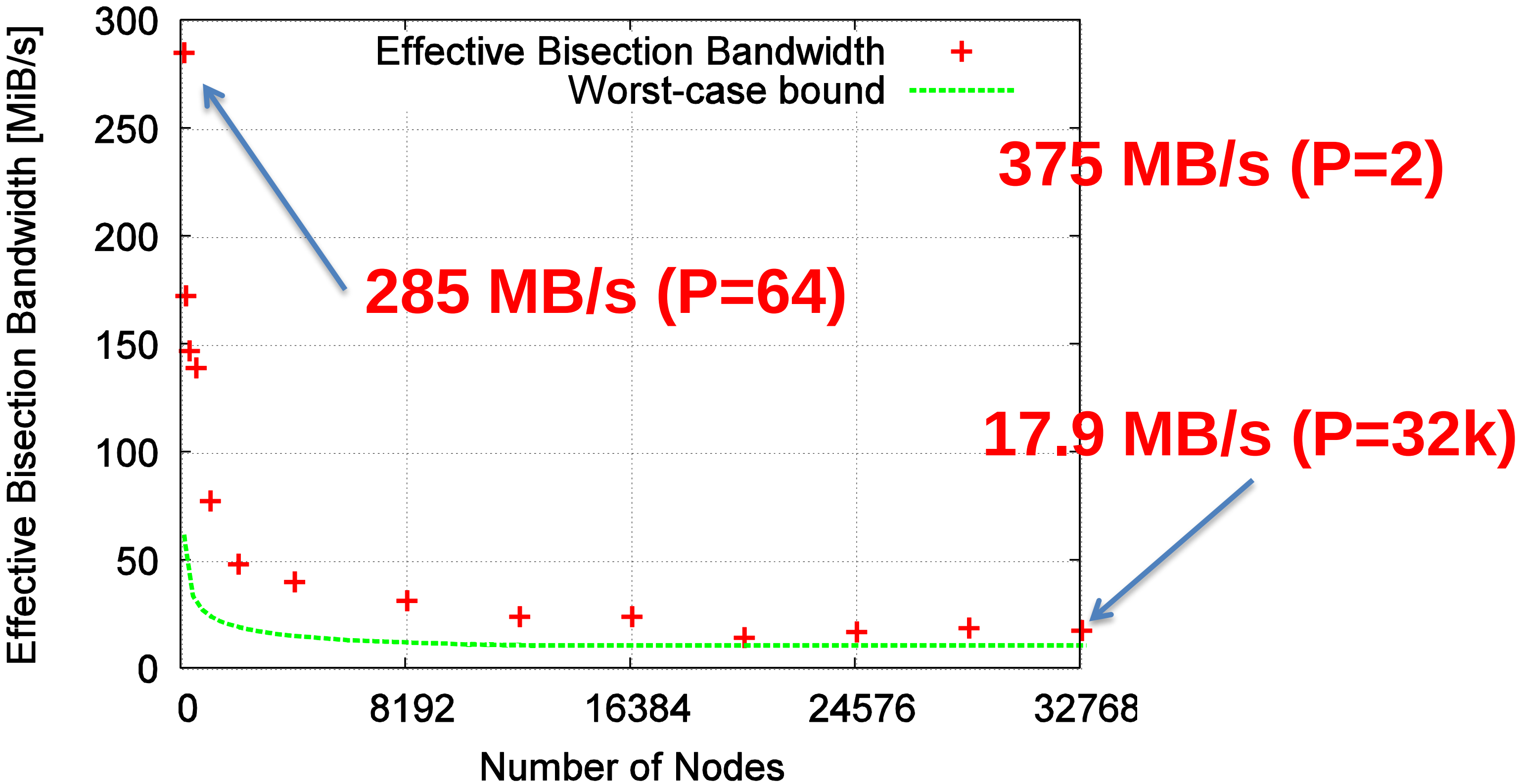
- R requests: $T_{match}(R) \leq 100ns \cdot R; \;\; T(13) \geq 1.3\mu s$
  - Benchmark: Netgauge/one_one_req_queue

[EuroMPI'10]: Hoefler et al.: "Toward Performance Models of MPI Implementations …"

Example: The not-so-ideal (but realistic) Case III

- Congestion is often ignored
  - Very hard to determine but worst-case can be calculated (assuming rectangular 3D Torus on BG/P)
  - effective Bisection Bandwidth
    - Average bandwidth of a random perfect matching
- Upper bound is congestion-less (see p2p model)
- Lower bound assumes worst-case mapping
  - Assume ideal adaptive routing (BG/P)
  - Congestion of $\mathcal{O}(\sqrt[3]{P})$ per link

Example: Worst-case vs. Average-case Congestion

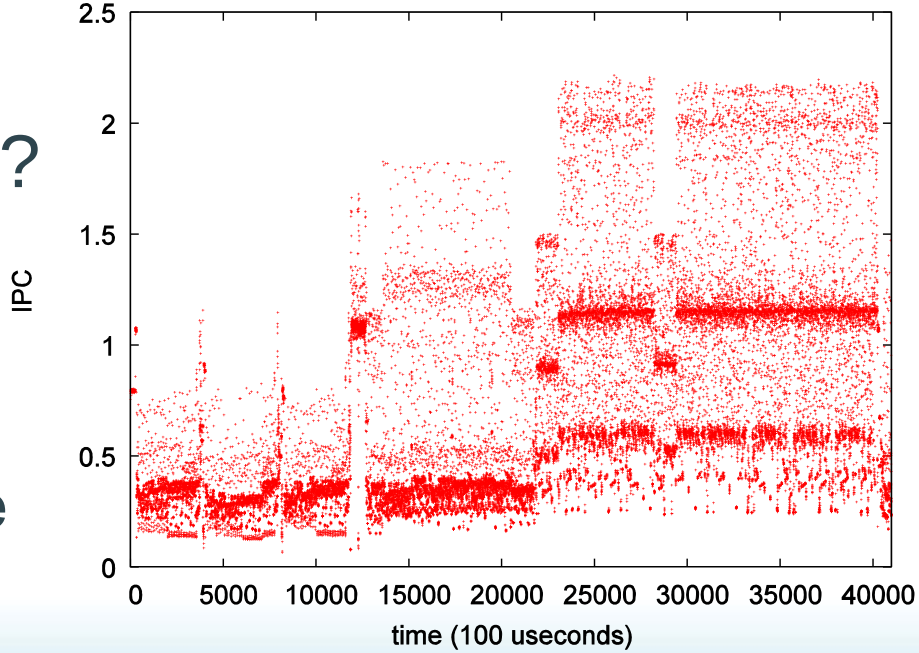


- Average seems to converge to worst-case (large P)
  - Benchmark: Netgauge/ebb

[EuroMPI'10]: Hoefler et al.: "Toward Performance Models of MPI Implementations …"

Tool 3: Modeling for Legacy Applications

- Current programming models don't support performance modeling well
  - Performance analysis tools to gather data
  - Costly manual analysis
- Automatic modeling tools?
  - Detection of regions
    - changes in IPC
  - Example: MILC, detect five "critical regions", same result as manual modeling



data collected with NCSA perfsuite/papi

Performance-centric Software Development

- Performance models allow to ***explain*** application performance
  - Find problems, not a solutions
  - Mostly a scientific exercise to *understand*
- Integrate modeling and the programming model to allow ***performance-centric design***
  - Understand *and* avoid problems by design
  - Structured approach to “Performance Engineering”

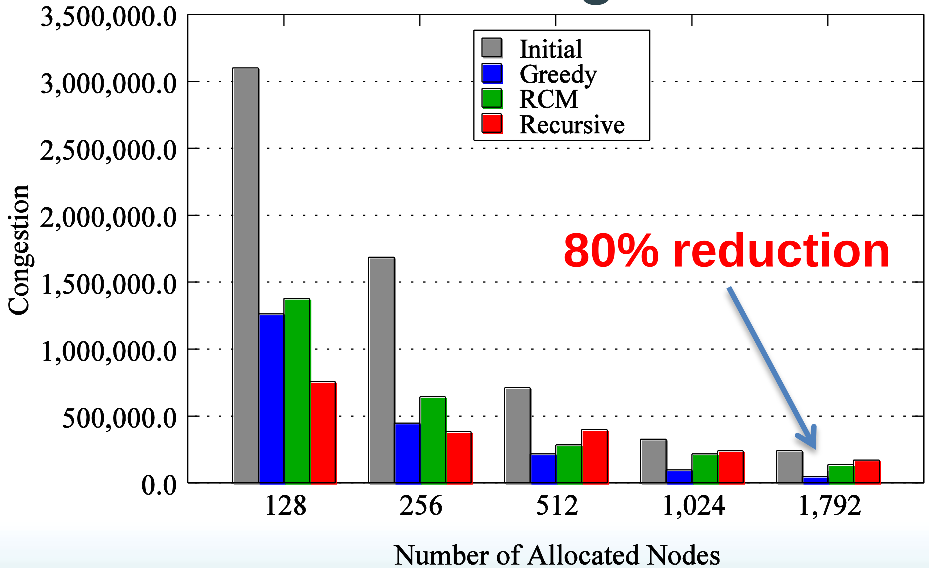
Tool 1: Performance-transparent Abstractions

- **Abstractions** allow for performance portability and ease of programming!
  - How to choose an abstraction? What to expect?
- Determine application requirements! → PM
  - e.g., nonblocking collectives, sparse collectives
- Trade-off between performance, portability, and programmability is most important!
- Performance must be **first class citizen** in HPC programming models (yet it isn't!)!

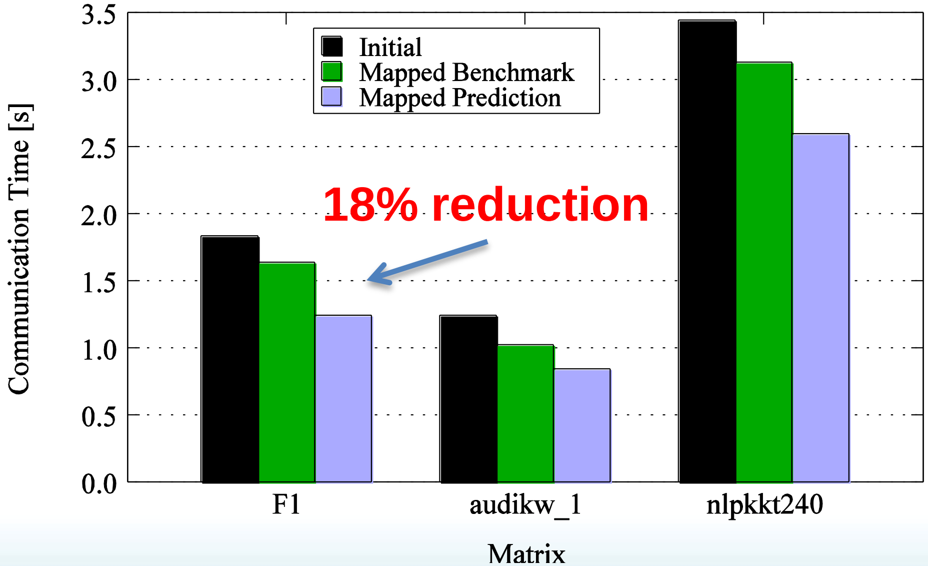
[PPL]: Balaji, Hoefler et al.: "MPI on Millions of Cores", [SciDAC'10] "MPI at Exascale"
[SC07]: Hoefler et al.: "Implementation and Performance Analysis of Non-Blocking Collective Operations for MPI"
[PPoPP'11,ISC'11]: Willcock, Hoefler et all. "Active Pebbles: Parallel Programming for Data-Driven Applications"

Tool 2: Model-driven Topology Mapping

- Can optimize performance significantly, nearly no impact on programmability (MPI-2.2 [CCPE])!
  - Computing a mapping is expensive!
  - Scalable algorithms in [ICS'11]



PERCS Network - simulated

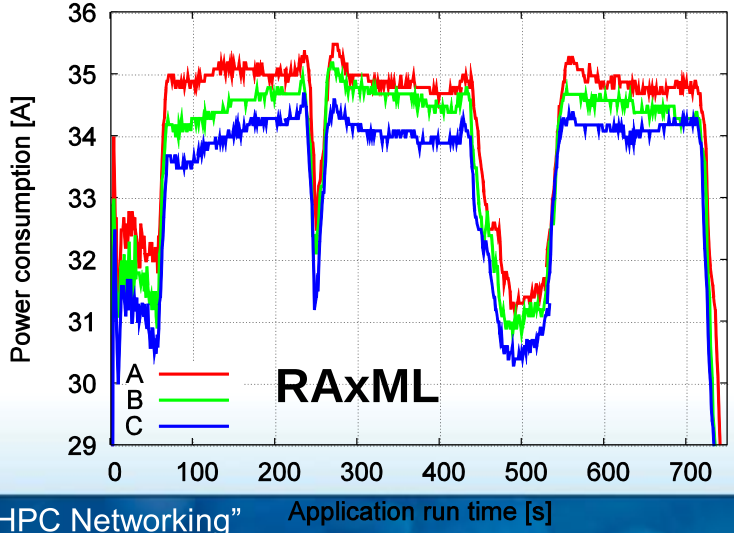


BG/P Network - measured

[ICS'11]: Hoefler and Snir: Generic Topology Mapping Strategies for Large-Scale Parallel Architectures
[CCPE]: Hoefler et al.: "The Scalable Process Topology Interface of MPI 2.2"

Tool 3 (Idea): Power-aware programming?

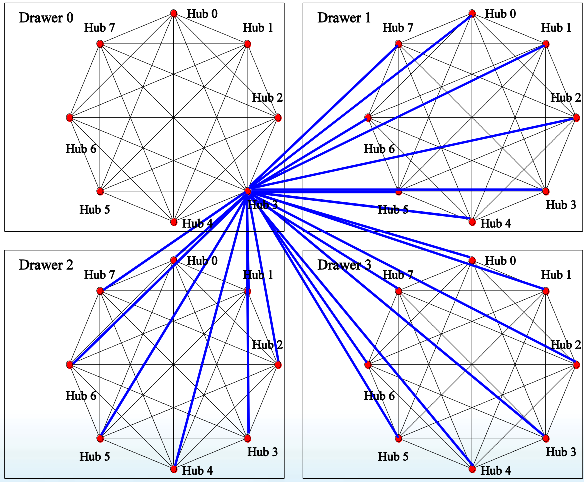
- Provide models and abstractions for power usage
  - Mostly data-movement centric
  - Flops-metric is not predictive for energy consumption
- But: performance and energy consumption correlate (finish faster = use less power)
  - detailed analysis for networks in [CiSE'10]



[CiSE'10]: Hoefler: "Software and Hardware Techniques for Power-Efficient HPC Networking"
[CAC'09]: Hoefler et al.: "A Power-Aware, Application-Based, Performance Study Of … Networks"

Tool 4: Model-guided System Design

- Systems and Applications need to evolve in parallel
  - Applications need to be ready when a machine goes online!
  - Co-design is attractive, models as “communication medium”
- Application-specific interconnection optimization:
  - Optimized general routing [IPDPS’11]
  - Application-specific routing
  - Novel topologies [HotI’10]
  - Reconfigurable architectures or topologies



[IPDPS'11]: Domke, Hoefler, Nagel: "Deadlock-Free Oblivious Routing for Arbitrary Topologies“
[HotI'10]: Arimilli, Hoefler et al.: "The PERCS High-Performance Interconnect"

Summarizing the Big Picture

- Develop performance modeling as a science discipline
  - *Observation, measurement, hypothesis, test*
  - Enables us to explain application performance
- Foster wide adoption of modeling techniques
  - Establish methodology, provide tool support
  - Static applications work, many open problems though
- Transform results into an engineering discipline
  - Not only explain performance but indicate how to program or tune code for best performance

References to Previous Work

[IPDPS'11]: Domke, Hoefler, Nagel: "Deadlock-Free Oblivious Routing for Arbitrary Topologies"

[PPL]: Balaji, Hoefler et al.: "MPI on Millions of Cores", [SciDAC'10] "MPI at Exascale"

[SIAM-CSE'10]: Gropp, Hoefler, Snir: "Performance Modeling for Systematic Performance Tuning"

[PROPER'10]: Hoefler: "Bridging Performance Analysis Tools and Analytic Performance Modeling"

[SC10]: Hoefler et al.: "Characterizing the Influence of System Noise … by Simulation" (Best Paper)

[CCPE]: Hoefler et al.: "The Scalable Process Topology Interface of MPI 2.2"

[HotI'10]: Arimilli, Hoefler et al.: "The PERCS High-Performance Interconnect"

[LSAP'10]: Hoefler et al.: "LogGOPSim – Simulating … Apps. in the LogGOPS Model" (Best Paper)

[PPoPP'10]: Hoefler et al.: "Scalable Communication … for Dynamic Sparse Data Exchange"

[PMEO'07]: Hoefler et al: "Low-Overhead LogGP Parameter Assessment …"

[HPCC'07]: Hoefler et al: "Netgauge: A Network Performance Measurement Framework"

[SC07]: Hoefler et al.: "Implementation and Performance Analysis of Non-Blocking Collective Operations for MPI“

[HPCNano’06]: Hoefler et al.: “Parallel scaling of Teter's minimization for Ab Initio calculations”